Surface X-Ray Analysis of 5-Chlorouracil on Ag(111)

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Introduction: The structure of the uracil-derivative 5-Chlorouracil (5-CLU) was investigated by surface x-ray diffraction (SXRD). Although the study of large organic molecules deposited on single crystal surfaces has become a major branch in surface science, detailed structure analyses determining the atomic coordinates in the unit cell are very rare. This is due to the large unit-cells, their low symmetry and sensitivity of the molecules. STM, LEED or SEXAFS often do not provide atomic resolution or have to surrender in case of too large unit cells. Previous SXRD analysis has shown that for 2-Thiouracil and end-capped quaterthiophene even on a weakly interacting substrate like Ag(111) bond lengths and angles can be significantly distorted [1]. Moreover, for 5-Iodouracil an adsorption-induced reaction was observed leading to the formation of 5-5'-Diuracil [2]. The aim of the experiment was to study the structure of 5-CLU, which is expected to be more stable than its higher homologues.

Methods and Materials: 5-CLU was deposited in situ on Ag (111) by evaporation from a Knudsen cell until a sharp six domain LEED pattern was visible. The Ag(111) reflections were considerably reduced in intensity indicating the possible formation of a multi-layer structure.

Results: In total 48 independent in-plane reflections and 6 superlattice rods were measured. 5-CLU forms an incommensurate superstructure which relative to the Ag(111)-(1x1) surface unit cell is described by the matrix $\begin{pmatrix} 5.0007 & 0.1379 \\ 0.0118 & 2.3572 \end{pmatrix}$ (unit cell with parameters: a_0 = 14.252Å, b_0 = 6.793Å, γ = 118.36°).

Conclusions: The Fig.1 shows the z-projected Patterson-function, P(u,v), calculated from the in-plane data. P(u,v) shows only three independent peaks of about the same height. The nearly hexagonal arrangement as well as the peak heights can be related to the bulk structure of 5-CLU [3], which is shown in the lower part of Fig.1. This structure was used as a starting model. Its basic features are parallel sheets of hydrogen bonded molecules. In Fig.1 two layers are shown. Molecules belonging to the upper and lower layer are indicated by (u) and (l), respectively. Using this model the Patterson peaks can be explained by the correlation between complete pyrimidine rings. We conclude that 5-CLU is stable. This is in contrast to 5-Iodouracil, which can be attributed to the stronger Cl-C bond as compared to the I-C bond. The full structure refinement on the basis of the in-plane data is so far compatible with this picture yielding an unweighted residual (R_u) of R=15 % for a four layer structure with identical x/y atom positions in the first and third molecule layer and second and fourth layer, respectively.

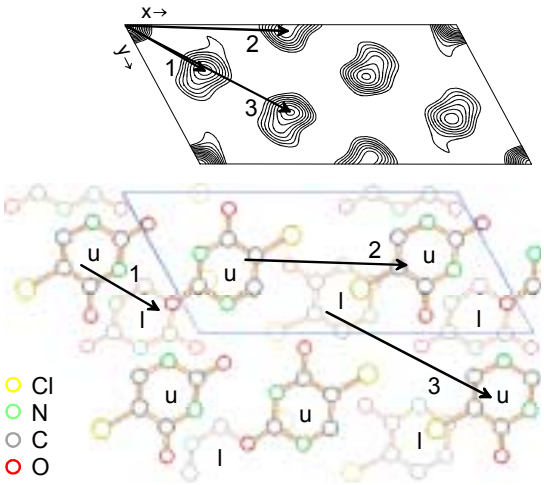

Fig. 1 Patterson-function P(u,v) of 5-CLU on Ag(111) (upper part) and z-projected model structure

From the superlattice rods showing a modulated structure a double or multilayer structure can also be inferred indicating a strong inter-layer interaction possibly mediated by the chlorine-atoms with the pyrimidine rings of the adjacent layers as in the bulk [3]. The data analysis is in progress.

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